

Spin polarization and edge currents in topological superconductors

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The spin character of topologically protected edge states in noncentrosymmetric superconductors is investigated through exact diagonalization of Bogoliubov-de Gennes Hamiltonians. We find that due to the spin-orbit coupling and parity-mixing, the edge states exhibit an intricate spin structure, which depends on the edge momentum. If the superconductor is brought into contact with a ferromagnetic insulator, the exchange field coupling to the spin-polarized edge states gives rise to a spontaneous edge current. We study the variation of the zero-temperature edge current on the magnetization direction and the singlet-triplet mixing in the superconductor, and show that it can exhibit singular dependence on the exchange-field strength.

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Introduction.—The realization that effectively noninteracting insulators and superconductors can be systematically classified in terms of their topological properties has inspired an intense research effort [1–4]. An important class of topological systems are noncentrosymmetric superconductors (NCSs), characterized by strong antisymmetric spin-orbit coupling (SOC) and a mixing of spin-singlet and spin-triplet pairing [5]. Remarkably, both fully gapped and nodal NCS can have nontrivial topology, which is manifested by topologically protected edge states via the bulk-boundary correspondence. In a fully gapped NCS, the edge states are dispersing Majorana modes [4, 6–8], whereas a nodal NCS exhibits nondispersing zero-energy edge states (flat bands) [9–14]. There are several candidate materials for topological NCSs, such as CePt₃Si [15], Li₂Pt₃B [16], and BiPd [17]. Furthermore, it has been proposed to engineer an NCS by exploiting the proximity effect in a material with strong SOC placed in contact with a topologically trivial superconductor [18–21], or in the metallic layer realized at oxide interfaces [22, 23].

In this Letter, we examine two contrasting examples of NCSs: (i) a fully gapped system with helical Majorana edge states and (ii) a nodal state with nondegenerate flat bands. We demonstrate that these edge states are strongly spin polarized, which originates from both the SOC and parity mixing in the superconductor. If the superconductor is brought into contact with a ferromagnetic insulator, the coupling to the exchange field alters the dispersion of these subgap states so that they carry a charge current along the edge. Besides the edge-state contribution, there is also a contribution to the edge current from bulk continuum states. We find that the properties of the edge current reflect the topological character of the NCS: For example, the topologically protected flat bands of the nodal NCS are responsible for a strong edge current with singular dependence on the exchange-field strength.

Model Hamiltonian.—Quasiparticle motion in an NCS is described by the Bogoliubov-de Gennes Hamiltonian $H = \sum_{\mathbf{k}} \Psi_{\mathbf{k}}^\dagger H_{\mathbf{k}} \Psi_{\mathbf{k}}$, with $\Psi_{\mathbf{k}} = (c_{\mathbf{k}\uparrow}, c_{\mathbf{k}\downarrow}, c_{-\mathbf{k}\uparrow}^\dagger, c_{-\mathbf{k}\downarrow}^\dagger)^T$ and

$$H_{\mathbf{k}} = \begin{pmatrix} \varepsilon_{\mathbf{k}} \sigma_0 - \lambda \mathbf{l}_{\mathbf{k}} \cdot \boldsymbol{\sigma} & \Delta_{\mathbf{k}} \\ \Delta_{\mathbf{k}}^\dagger & -\varepsilon_{\mathbf{k}} \sigma_0 + \lambda \mathbf{l}_{\mathbf{k}} \cdot \boldsymbol{\sigma}^* \end{pmatrix}, \quad (1)$$

where $\mathbf{l}_{\mathbf{k}} = \hat{\mathbf{x}} \sin k_y - \hat{\mathbf{y}} \sin k_x$, $\varepsilon_{\mathbf{k}} = t(\cos k_x + \cos k_y) - \mu$, and $\Delta_{\mathbf{k}} = (\psi_{\mathbf{k}} \sigma_0 + \mathbf{d}_{\mathbf{k}} \cdot \boldsymbol{\sigma})(i\sigma_y)$. Here, $c_{\mathbf{k}\sigma}^\dagger$ denotes the electron creation operator with spin σ and momentum \mathbf{k} , μ represents the chemical potential, t is twice the nearest-neighbor hopping integral, λ stands for the SOC strength, and $\boldsymbol{\sigma}$ denotes the vector of Pauli matrices. The even-parity spin-singlet and odd-parity spin-triplet components of the superconducting order parameter are parametrized as $\psi_{\mathbf{k}} = \Delta_0 f(\mathbf{k}) q$ and $\mathbf{d}_{\mathbf{k}} = \Delta_0 f(\mathbf{k}) \mathbf{l}_{\mathbf{k}} (1 - q)$, respectively. With the parameter q , the NCS can be tuned from purely spin-triplet ($q = 0$) to purely spin-singlet ($q = 1$) pairing. The structure factor $f(\mathbf{k})$ allows to study different orbital-angular-momentum pairing states. In the following we consider two cases: (i) $f(\mathbf{k}) = 1$ for an NCS with $(s+p)$ -wave pairing symmetry and (ii) $f(\mathbf{k}) = \sin k_x \sin k_y$ for the so-called $(d_{xy}+p)$ -wave pairing state. In our numerical calculations we choose $(t, \mu, \lambda, \Delta_0) = (4.0, 4.0, -2.0, 0.5)$.

Edge states.—To examine the different topological properties of $(s+p)$ -wave and $(d_{xy}+p)$ -wave pairing states, we study first the subgap states at the edge of the NCS, both with and without a proximity-induced exchange field \mathbf{H}_{ex} acting on the leading edge. To that end, we compute the spin- and momentum-resolved density of states (DOS) of Hamiltonian (1) in a ribbon geometry with edges perpendicular to the (10) direction. The momentum-resolved DOS and the spin-resolved DOS in the n -th layer from the edge are given by

$$\rho_n(E, k_y) = -\frac{1}{4\pi} \text{Im} \left[\text{Tr} \left\{ G_{k_y}^{(10)}(n, n; E) \right\} \right], \quad (2a)$$

$$\rho_n^\mu(E, k_y) = -\frac{\hbar}{4\pi} \text{Im} \left[\text{Tr} \left\{ S^\mu G_{k_y}^{(10)}(n, n; E) \right\} \right], \quad (2b)$$

respectively, where $S^\mu = \text{diag}(\sigma^\mu, -[\sigma^\mu]^*)$. Here, $G_{k_y}^{(10)} = (E + i\eta - H_{k_y}^{(10)})^{-1}$ denotes the zero-temperature lattice Green's function of the ribbon with $H_{k_y}^{(10)} = \frac{1}{2\pi} \int dk_x e^{ik_x(n-n')} H_{\mathbf{k}} + \delta_{n',1} \delta_{n,1} \text{diag}(\mathbf{H}_{\text{ex}} \cdot \boldsymbol{\sigma}, -[\mathbf{H}_{\text{ex}} \cdot \boldsymbol{\sigma}]^T)$. The expressions in Eqs. (2) are evaluated by taking a ribbon of width up to $N = 10^3$ and an intrinsic broadening $\eta = 0.005$.

We first discuss the edge DOS for $\mathbf{H}_{\text{ex}} = 0$. Figure 1 shows the local DOS at the (10) edge integrated over the ten outermost layers, i.e., $\sum_{n=1}^{10} \rho_n(E, k_y)$, for the triplet-dominated

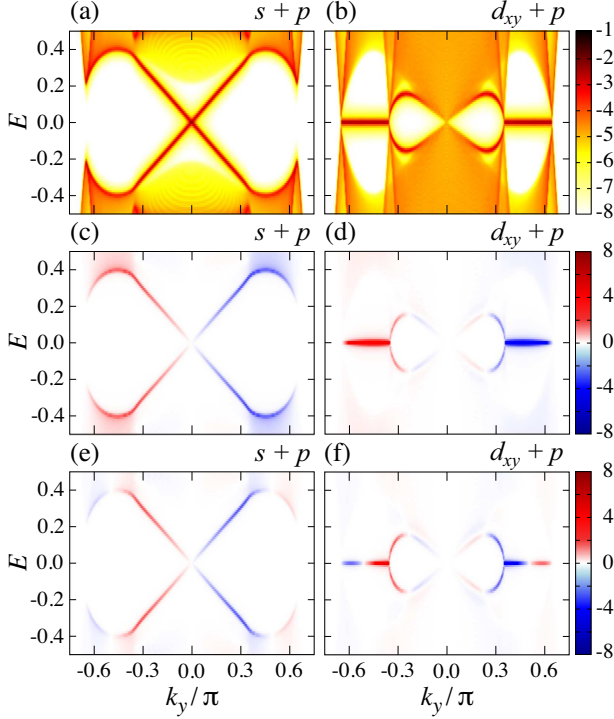


FIG. 1. (a) and (b): Momentum-resolved DOS on a log scale for the ten outermost layers at the (10) edge of an $(s+p)$ -wave and a $(d_{xy}+p)$ -wave NCS, respectively. (c), (d) x component and (e), (f) z component of the spin-resolved DOS for the outermost layer at the (10) edge in units of $\hbar/10$ on a linear scale. In all cases we choose $q = 0.25$, representative for the triplet-dominated pairing state.

pairing state. Ten layers are on the order of the superconducting coherence length, i.e., the distance over which the edge states are localized. Here, we present the edge DOS only for the triplet-dominated phase; the edge DOS for the singlet-dominated phase is included as Fig. 6 in the Supplemental Material (SM) for completeness. Figures 1 and 6 reveal both the subgap states (dark red) and the bulk continuum states (orange and yellow). In the parameter ranges $q < q_{c,L} \simeq 0.472$ and $q > q_{c,U} \simeq 0.583$, the $(s+p)$ -wave state is a fully gapped superconductor in symmetry class DIII. For $q < q_{c,L}$, the superconductor has a topologically nontrivial character with a non-zero \mathbb{Z}_2 topological number [2, 8, 25]. By the bulk-boundary correspondence, we accordingly find helical Majorana subgap states, see Fig. 1(a) [6–8]. For $q > q_{c,U}$, the system is topologically trivial and the subgap states hence disappear [24]. The $(d_{xy}+p)$ -wave NCS, in contrast, is nodal and therefore does not have a quantized global topological number for any q . However, by treating every point in the edge Brillouin zone (BZ) as the edge of a one-dimensional system, one can define a momentum-dependent winding number $W_{(10)}(k_y)$, which only changes across projected nodes of the bulk gap [10–13]. Provided that $q \notin [q_{c,L}, q_{c,U}]$, one finds $W_{(10)}(k_y) = \pm 1$ for $|k_y| \in [k_{F,+}, k_{F,-}] \simeq [0.352\pi, 0.648\pi]$. That is, when k_y lies between the projected edges $k_{F,+}$ and $k_{F,-}$ of the two spin-orbit-split Fermi surfaces, the winding number $W_{(10)}(k_y)$

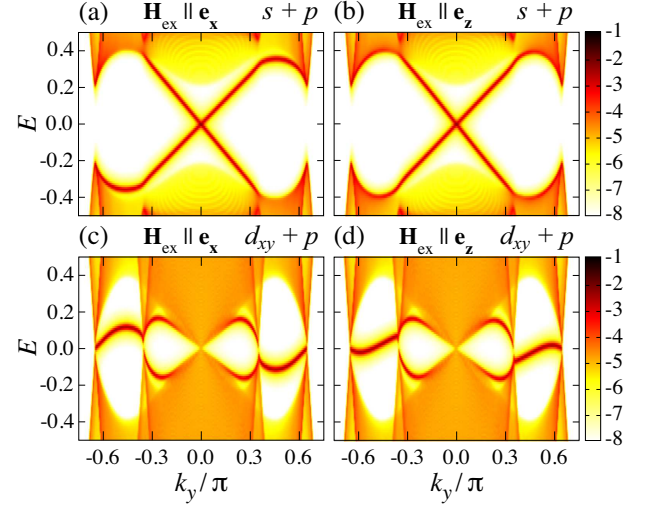


FIG. 2. (Color online) Surface DOS on a log scale for the ten outermost layers at the (10) edge of an $(s+p)$ -wave and a $(d_{xy}+p)$ -wave NCS in the presence of an exchange field in the leading edge with magnitude $h_{\text{ex}} = 0.4$. (a) and (c): exchange field along the x axis. (b) and (d): exchange field along the z axis. As in Fig. 1, we choose $q = 0.25$, representative for the triplet-dominated pairing state.

takes on the nonzero values ± 1 , which ensures the existence of nondegenerate zero-energy flat bands at these momenta k_y [9]. For $|k_y| < k_{F,+}$, on the other hand, there are topologically trivial dispersing states for $q < q_{c,L}$, and doubly degenerate zero-energy states with $W_{(10)}(k_y) = \pm 2$ for $q > q_{c,U}$, see Figs. 1(b) and 6(b).

In the lower two rows of Fig. 1, we present the spin-resolved edge DOS $\rho_{n=1}^\mu(E, k_y)$ in the absence of an exchange field. The corresponding plots for the singlet-dominated phase are given in Fig. 6 in the SM. Interestingly, both the continuum and subgap states show a strong polarization in the xz spin-plane, but a vanishing y component. The magnitude and sign of the spin polarization are strongly momentum dependent, and display a complicated interplay between singlet-triplet ratio q and SOC strength λ . For example, for the $(s+p)$ -wave state, we find that the x -spin polarization in the band with the smaller gap can reverse sign near the edge of the larger gap. In contrast, the nondegenerate zero-energy flat bands of the $(d_{xy}+p)$ -wave NCS exhibit a strong and robust x -spin polarization, whereas the z -spin polarization is smaller and changes sign close to $\pm(k_{F,-} - k_{F,+})/2$. The doubly degenerate states for $(d_{xy}+p)$ -wave pairing with $q > q_{c,U}$ give opposite contributions to the spin-resolved DOS of unequal magnitude, overall leading to a weaker spin polarization than for the nondegenerate states. As required by time-reversal symmetry, subgap states with opposite edge momenta have opposite spin polarizations. In the case of the $(s+p)$ -wave state, this ensures the robustness of the linearly dispersing edge states against backscattering from nonmagnetic impurities. On the other hand, in the $(d_{xy}+p)$ -wave NCS this leads to a considerable suppression of time-reversal-symmetric scat-

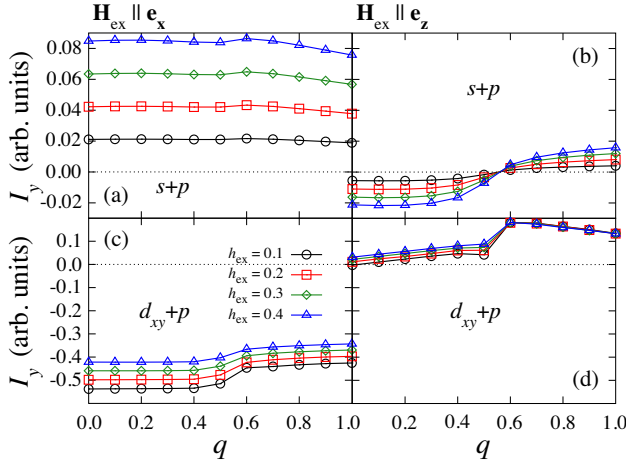


FIG. 3. (Color online) Edge current I_y as a function of singlet-triplet parameter q for various exchange-field strengths h_{ex} in an NCS with an exchange field in the leading edge. Top row: $(s+p)$ -wave NCS and exchange field along (a) the x axis and (b) the z axis. Bottom row: $(d_{xy}+p)$ -wave NCS and exchange field along (c) the x axis and (d) the z axis.

tering processes connecting the oppositely x -spin-polarized flat bands for $k_y > 0$ and $k_y < 0$.

The nontrivial spin character of the edge states and the resulting absence of certain scattering processes could be tested experimentally using Fourier-transform scanning tunneling spectroscopy. Another possibility is to probe the spin polarization of the subgap states by bringing the NCS into contact with a ferromagnetic insulator. It is expected that the proximity-induced exchange field \mathbf{H}_{ex} will lead to a perturbative correction to the energy of the spin-polarized edge states proportional to $\sum_{\mu=1}^3 H_{\text{ex}}^{\mu} \rho_n^{\mu}(E, k_y)$. Since the flat-band states at $+k_y$ and $-k_y$ are oppositely spin polarized, the coupling to the exchange field will shift the energy of these edge states in opposite directions. To test this expectation, we show in Fig. 2 the edge band structure in the triplet-dominated phase in the presence of an exchange field of magnitude $h_{\text{ex}} = |\mathbf{H}_{\text{ex}}| = 0.4$ acting on the leading edge. (The corresponding plot for the singlet-dominated phase is given as Fig. 7 in the SM.) Indeed, the edge states of both the $(s+p)$ -wave and $(d_{xy}+p)$ -wave NCS display a linear shift in energy, which is to a good approximation proportional to $\sum_{\mu=1}^3 H_{\text{ex}}^{\mu} \rho_1^{\mu}(E, k_y)$, as long as $h_{\text{ex}} \lesssim \Delta_0$. The doubly degenerate flat bands that occur for $q > q_{c,U}$ in the $(d_{xy}+p)$ -wave NCS split due to the opposite spin polarization of the two degenerate states, see SM.

Edge Currents.—The energy shifts of the edge states due to the coupling to the exchange field can give rise to a spontaneous edge charge current. To evaluate this current, we define new electron operators in mixed real- and momentum-space $c_{nk_y\sigma} = \frac{1}{\sqrt{2\pi L_x}} \sum_{k_x} c_{\mathbf{k}\sigma} e^{-ik_x n}$, where n represents the layer index and L_x denotes the width of the ribbon. With this, the layer-dependent current operator along the y axis can be expressed as $j_n = -\frac{e}{\hbar} \frac{1}{N_y} \sum_{k_y} [j_{n,k_y}^{(1)} + j_{n,k_y}^{(2)}]$, where N_y is the

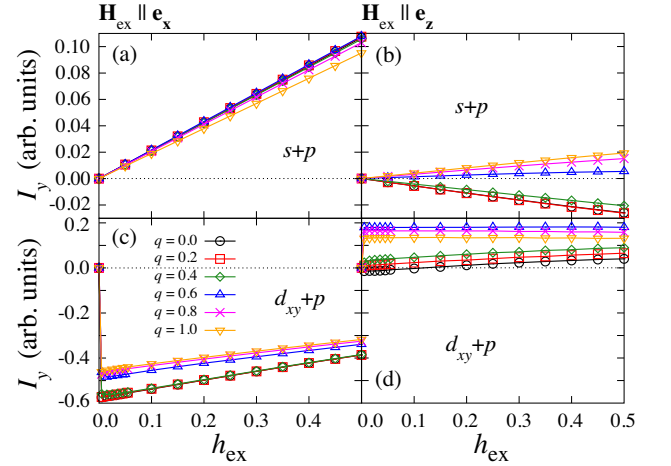


FIG. 4. (Color online) Edge current I_y as a function of exchange-field strength h_{ex} for various values of the singlet-triplet parameter q . Top row: $(s+p)$ -wave NCS and exchange field along (a) the x axis and (b) the z axis. Bottom row: $(d_{xy}+p)$ -wave NCS and exchange field along (c) the x axis and (d) the z axis.

number of k_y points in the edge BZ and

$$j_{n,k_y}^{(1)} = -t \sin k_y \left(c_{nk_y\uparrow}^{\dagger} c_{nk_y\uparrow} + c_{nk_y\downarrow}^{\dagger} c_{nk_y\downarrow} \right), \quad (3a)$$

$$j_{n,k_y}^{(2)} = +\lambda \cos k_y \left(c_{nk_y\downarrow}^{\dagger} c_{nk_y\uparrow} + c_{nk_y\uparrow}^{\dagger} c_{nk_y\downarrow} \right). \quad (3b)$$

The contribution $j_{n,k_y}^{(1)}$ corresponds to nearest-neighbor hopping, whereas $j_{n,k_y}^{(2)}$ is due to SOC. We calculate the expectation value of the edge current at zero temperature from the spectrum E_{l,k_y} and the wavefunctions $|\psi_{l,k_y}\rangle$ of $H_{k_y}^{(10)}$,

$$I_y = -\frac{e}{\hbar} \frac{1}{N_y} \sum_{k_y} \sum_{l=1,2} \sum_{n=1}^{L_x/2} \sum_{l, E_l < 0} \langle \psi_{l,k_y} | j_{n,k_y}^{(\iota)} | \psi_{l,k_y} \rangle. \quad (4)$$

We observe that the current operators Eq. (3) are unaffected by the presence of the superconducting gaps or the edge; these only enter into Eq. (4) through the eigenstates $|\psi_{l,k_y}\rangle$.

In Figs. 3 and 4 we plot the edge current I_y as a function of singlet-triplet parameter q and exchange-field strength h_{ex} . Note that the current reverses sign with the direction of the exchange field. For both the $(s+p)$ -wave and $(d_{xy}+p)$ -wave cases, we indeed find spontaneous currents flowing along the edge of the NCS. However, the currents in the two cases are dramatically different. For weak to moderate exchange-field strengths, the magnitude of the currents in the $(s+p)$ -wave state is always small compared to the $(d_{xy}+p)$ -wave case. The current at the edge of the $(s+p)$ -wave NCS grows linearly with the exchange field as long as $h_{\text{ex}} \lesssim \Delta_0$, see Figs. 4(a) and 4(b). On the other hand, in the $(d_{xy}+p)$ -wave NCS, the current exhibits a remarkable deviation from linear behavior: At zero temperature, an infinitesimally small exchange field is sufficient to generate a large current in the NCS, as seen in Figs. 4(c) and 4(d). The currents in both the $(s+p)$ -wave

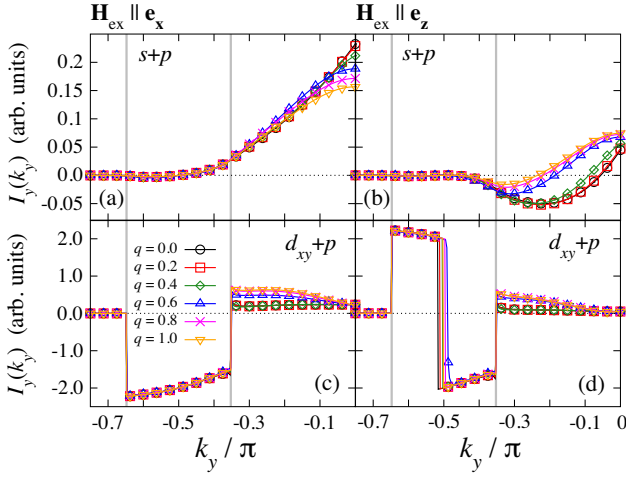


FIG. 5. (Color online) Momentum-resolved edge current $I_y(k_y)$ for various values of singlet-triplet parameter q . Top row: $(s+p)$ -wave NCS and exchange field along (a) the x axis and (b) the z axis. Bottom row: $(d_{xy}+p)$ -wave NCS and exchange field along (c) the x axis and (d) the z axis. The exchange field is $h_{\text{ex}} = 0.2$. The vertical gray lines indicate the projections of the edges of the two spin-orbit-split Fermi surfaces.

and $(d_{xy}+p)$ -wave NCSs depend only weakly on q for both $q < q_{c,L}$ and $q > q_{c,U}$. However, in the $(s+p)$ -wave NCS and for an exchange field along the z axis, the current changes sign as the pairing state is tuned from triplet dominated to singlet dominated. In the $(d_{xy}+p)$ -wave state, on the other hand, the current always shows a clear change in magnitude as one goes from $q < q_{c,L}$ to $q > q_{c,U}$, see Figs. 3(c) and 3(d).

To gain a better understanding of the origin of the currents, it is instructive to examine the current $I_y(k_y)$ contributed by states at $+k_y$ and $-k_y$, i.e., the even part of the k_y -summand in Eq. (4). In Fig. 5, we show the evolution of $I_y(k_y)$ with the singlet-triplet parameter q for exchange fields along the x and z axes. For the $(s+p)$ -wave pairing state, this reveals that the edge current is predominantly due to states with $|k_y| < k_{F,+}$, whereas in the $(d_{xy}+p)$ -wave NCS the current originates mostly from states with $k_{F,+} < |k_y| < k_{F,-}$. Interestingly, for an exchange field along the x axis the current shows no variation with q in this momentum range and is independent of the exchange-field strength (not shown). The k_y -resolved current for the z -polarized exchange field in Fig. 5(d) shows similar characteristics, but also a jump in $I_y(k_y)$ at the location of the sign change of the z component of the spin polarization of the nondegenerate edge states, cf. Fig. 1(f).

Discussion.—The remarkably strong edge current in the $(d_{xy}+p)$ -wave NCS directly follows from the coupling of the exchange field to the nondegenerate flat bands of the NCS. Inspection of Eq. (3) shows that the hopping part of the momentum-resolved current is proportional to the difference in the number of states below the Fermi energy at $+k_y$ and $-k_y$, whereas the spin-orbit part is proportional to the sum of the x -spin polarization at these momenta. Thus, even for an infinitesimal field, the opposite energy shift of the oppositely

x -spin-polarized nondegenerate flat bands yields a large contribution to the current, which is approximately

$$I_y \simeq \frac{e}{\hbar} \int_{k_{F,+}}^{k_{F,-}} \frac{dk_y}{2\pi} \text{sgn} \left[\sum_{\mu} H_{\text{ex}}^{\mu} \rho_1^{\mu}(0, k_y) \right] \times \left(-t \sin k_y + \lambda \sum_{n=1}^{L_x/2} \rho_n^x(0, k_y) \cos k_y \right). \quad (5)$$

The sign of the edge-state spin polarization along the exchange-field direction thus plays a critical role in generating the current, and explains the jump in the momentum-resolved current for the z -polarized exchange field. We observe that for the $(d_{xy}+p)$ -wave NCS, states with $|k_y| \notin [k_{F,+}, k_{F,-}]$ only contribute to the current through the SOC coupling, while in the $(s+p)$ -wave pairing phase the hopping contribution is zero for all k_y , since in both cases the number of states below the Fermi energy at $+k_y$ and $-k_y$ are always equal. The splitting of the doubly degenerate flat bands in the majority-singlet $(d_{xy}+p)$ -wave NCS can nevertheless produce a sizeable current, as the shifting of the negatively (positively) spin-polarized states below (above) the Fermi energy generates a finite x -spin polarization and hence a current via the spin-orbit coupling. This accounts for the change in the current between $q < q_{c,L}$ and $q > q_{c,U}$ seen in Figs. 4(c) and (d).

Experimental detection of the edge currents should be possible in spite of the Meissner effect, which implies that screening currents exactly compensate the edge currents in a large sample. However, whereas the edge-current density decays into the bulk on the scale of the coherence length ξ_0 , the screening only builds up over the scale of the penetration depth λ_L . For an extreme type-II superconductor, characteristic of many NCSs [5], the screening currents will therefore be suppressed in a sample of width W with $\xi_0 \ll W \ll \lambda_L$. This argument also holds for an engineered NCS. We note that an edge current is also induced by placing the NCS in contact with a ferromagnetic metal [26].

Summary.—We have shown that the subgap edge states of an NCS are typically strongly spin polarized, which we have illustrated for two model NCS with distinct topological properties, specifically the fully gapped $(s+p)$ -wave and the nodal $(d_{xy}+p)$ -wave states. We have demonstrated that the presence of an exchange field in the outermost layer generates an edge current in the NCS. This is most clearly realized in the $(d_{xy}+p)$ -wave NCS, where the nondegenerate flat bands acquire a weak dispersion that leads to a strong edge current and to a singular dependence on the exchange-field strength. The remarkable current characteristics are a novel signature of these topologically protected states.

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Supplemental Material

Supplemental Figures

In Fig. 6 we plot the edge DOS and the x and z component of the spin-resolved edge DOS for an $(s+p)$ -wave and a $(d_{xy}+p)$ -wave NCS with singlet-dominated pairing state ($q = 0.75$). This should be compared to the triplet-dominated case shown in Fig. 1. Both the continuum and subgap states have a strong spin polarization, which is an odd function of edge momentum k_y , as required by time-reversal symmetry. The nondegenerate zero-energy flat bands of the $(d_{xy}+p)$ -wave NCS show a particularly strong and robust x -spin polarization, with a weaker z -spin polarization that changes sign near $\pm(k_{F,-} - k_{F,+})/2$. The doubly degenerate states of the $(d_{xy}+p)$ -wave NCS, which appear in the region $|k_y| \in [k_{F,+}, k_{F,-}]$, give opposite contributions to the spin-resolved DOS of unequal magnitude. They therefore exhibit a weaker overall spin polarization than the nondegenerate states. For the same value $q = 0.75$, i.e., also for the singlet-dominated pairing state, Fig. 7 displays the energy- and momentum-resolved edge band structure in the presence of a proximity-induced exchange field \mathbf{H}_{ex} in the leading edge. The coupling to the exchange field shifts the nondegenerate flat bands in opposite directions for $k_y > k_{F,+}$ and $k_y < -k_{F,+}$ and splits the doubly degenerate bands for $|k_y| < k_{F,+}$.

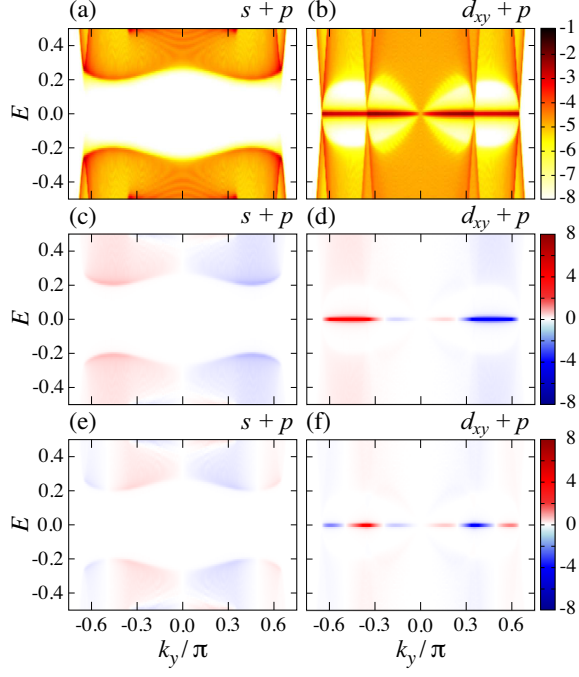


FIG. 6. (a) and (b) Energy- and momentum-resolved DOS on a log scale for the ten outermost layers at the (10) edge of an $(s+p)$ -wave and $(d_{xy}+p)$ -wave NCS, respectively. (c), (d) x component and (e), (f) z component of the spin-resolved DOS for the outermost layer at the (10) edge in units of $\hbar/10$ on a linear scale. We present typical results for the singlet-dominated pairing state with $q = 0.75$.

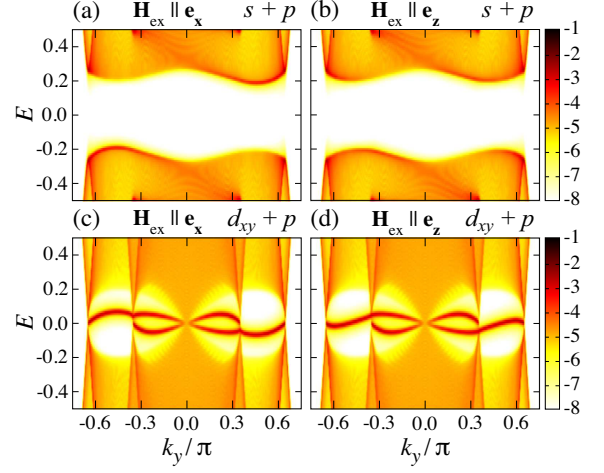


FIG. 7. Energy- and momentum-resolved edge DOS on a log scale for the ten outermost layers at the (10) edge of an $(s+p)$ -wave and $(d_{xy}+p)$ -wave NCS in the presence of an exchange field in the leading edge with magnitude $h_{\text{ex}} = 0.4$. (a) and (c): exchange field along the x axis. (b) and (d): exchange field along the z axis. We present typical results for the singlet-dominated pairing state with $q = 0.75$.